Jet Propulsion Laboratory
California Institute of Technology

Generalized Radiative Transfer as an Efficient Computational Tool for Spatial and/or Spectral Integration over Unresolved Variability in Multi-Angle Observations

Anthony B. Davis, Feng Xu, David J. Diner

AGU 2017 Fall Meeting, New Orleans, LA, 10-15 December, 2017
Special session: *Light Scattering and Radiative Transfer: Basic Research & Applications*

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Generalized Radiative Transfer *(GRT)* as an Efficient Computational Tool for Spatial and/or Spectral Integration over Unresolved Variability in Multi-Angle Observations *… of Aerosols*

-Yet-Accurate

Anthony B. Davis, ***Feng Xu, David J. Diner***

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Roadmap

- **Formulation of GRT**
  - Now with time/path dependence as well
  - Going from time-domain to absorption by a uniform gas
- **Motivation of GRT …**
  - as a resource for integration over *spatial* variability
  - as a resource for integration over *spectral* variability
- **Application to multi-angle observations of *optically thin* aerosol layers with interstitial (gaseous) absorption:**
  - Spatially variable scene, quasi-monochromatic sensor;
  - Spatially uniform scene, realistic spectral integration;
  - Both spatial and spectral variability.
- **Summary & Outlook**

Formulation of *standard* RT in plane-parallel media

$$\underbrace{\left(\frac{\partial}{\partial ct} + \mu\frac{\partial}{\partial z}\right) I + \sigma I}_{\text{sinks}} = \underbrace{S(ct, z, \boldsymbol{\Omega}) + q(ct, z, \boldsymbol{\Omega})}_{\text{sources}}$$

$$\mu = \Omega_z$$

Formulation of *standard* RT in plane-parallel media

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$$\mu = \Omega_z$$

Boundary/initial conditions:

$$I(ct, 0, \mathbf{\Omega}) \equiv 0 \text{ for } \mu > 0, \text{ and } I(ct, H, \mathbf{\Omega}) \equiv 0 \text{ for } \mu < 0;\ ct > 0$$

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Source *term*:

$$q(ct,z,\boldsymbol{\Omega}) = 2F_0\delta(ct)\delta(z)\delta(\boldsymbol{\Omega}-\boldsymbol{\Omega}_0)$$

Source *function*:

$$S(ct,z,\boldsymbol{\Omega}) = \sigma_\mathrm{s}\int_\Xi p(\boldsymbol{\Omega}\cdot\boldsymbol{\Omega}')I(ct,z,\boldsymbol{\Omega}')\mathrm{d}\boldsymbol{\Omega}'$$

Formulation of *standard* RT in plane-parallel media

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Source *function*: $S(ct,z,\mathbf{\Omega}) = \sigma_s \int_{\Xi} p(\mathbf{\Omega}\cdot\mathbf{\Omega}')I(ct,z,\mathbf{\Omega}')\mathrm{d}\mathbf{\Omega}'$

Integro-differential formulation: *Complete!*

NB. In this study: $\sigma = \sigma_s + \sigma_a = \omega_0\sigma_p + [(1-\omega_0)\sigma_p + \sigma_g]$

… later on: $\sigma_g \rightarrow k_\lambda$

Formulation of *standard* RT in plane-parallel media

Integral formulation:

Source *term*: $$q(ct, z, \mathbf{\Omega}) = 2F_0\delta(ct)\delta(z)\delta(\mathbf{\Omega} - \mathbf{\Omega}_0)$$

Source *function*: $$S(ct, z, \mathbf{\Omega}) = \sigma_\mathrm{s} \int_\Xi p(\mathbf{\Omega} \cdot \mathbf{\Omega}')I(ct, z, \mathbf{\Omega}')\mathrm{d}\mathbf{\Omega}'$$

"Formal" solution:

$$I(ct, z, \mathbf{\Omega}) = \begin{cases} \int_0^{ct} \int_0^{z} [S+q](ct', z', \mathbf{\Omega}) \mathrm{e}^{-\sigma \frac{z-z'}{\mu}} \delta\left((ct - ct') - \frac{z-z'}{\mu}\right) \frac{\mathrm{d}z'}{\mu} \mathrm{d}ct' & \text{for } \mu > 0 \\ \int_0^{ct} \int_z^{H} [S+q](ct', z', \mathbf{\Omega}) \mathrm{e}^{-\sigma \frac{z'-z}{|\mu|}} \delta\left((ct - ct') - \frac{z'-z}{|\mu|}\right) \frac{\mathrm{d}z'}{|\mu|} \mathrm{d}ct' & \text{for } \mu < 0 \end{cases}$$

Formulation of *standard* RT in plane-parallel media

"Ancillary" integral formulation:

Source *term*: $q(ct, z, \mathbf{\Omega}) = 2F_0\delta(ct)\delta(z)\delta(\mathbf{\Omega} - \mathbf{\Omega}_0)$

Source *function*: $S(ct, z, \mathbf{\Omega}) = \sigma_\mathrm{s} \int_\Xi p(\mathbf{\Omega} \cdot \mathbf{\Omega}')I(ct, z, \mathbf{\Omega}')\mathrm{d}\mathbf{\Omega}'$

Formal solution:

$$I(ct, z, \mathbf{\Omega}) = \begin{cases} \int_0^{ct}\int_0^{z}[S+q](ct', z', \mathbf{\Omega})\mathrm{e}^{-\sigma\frac{z-z'}{\mu}}\delta\left((ct-ct') - \frac{z-z'}{\mu}\right)\frac{\mathrm{d}z'}{\mu}\mathrm{d}ct' & \text{for } \mu > 0 \\ \int_0^{ct}\int_z^{H}[S+q](ct', z', \mathbf{\Omega})\mathrm{e}^{-\sigma\frac{z'-z}{|\mu|}}\delta\left((ct-ct') - \frac{z'-z}{|\mu|}\right)\frac{\mathrm{d}z'}{|\mu|}\mathrm{d}ct' & \text{for } \mu < 0 \end{cases}$$

Formulation of *generalized* RT in plane-parallel media

Equivalently, when $\left|\dot{T}(\tau)\right| = T(\tau) = \mathrm{e}^{-\tau}$ (Beer's law):

$$S(ct,z,\mathbf{\Omega}) = \int_0^{ct}\int_0^{H}\int_{\Xi} \mathcal{K}(ct,z,\mathbf{\Omega};ct',z',\mathbf{\Omega}')S(ct',z',\mathbf{\Omega}')\mathrm{d}\mathbf{\Omega}'\mathrm{d}z'\mathrm{d}ct' + Q_S(ct,z,\mathbf{\Omega})$$

with

kernel:
$$\mathcal{K}(ct,z,\mathbf{\Omega};ct',z',\mathbf{\Omega}') = \frac{\langle\sigma_\mathrm{s}\rangle}{|\mu'|}\Theta\left(\frac{z-z'}{\mu'}\right)\left|\dot{T}\left(\langle\sigma\rangle\frac{z-z'}{\mu'}\right)\right| \delta\left((ct-ct')-\frac{z-z'}{\mu'}\right)p(\mathbf{\Omega}\cdot\mathbf{\Omega}'),$$

source:
$$Q_S(ct,z,\mathbf{\Omega}) = F_0\delta\left(ct-\frac{z}{\mu_0}\right)\left|\dot{T}\left(\langle\sigma\rangle\frac{z}{\mu_0}\right)\right|\langle\sigma_\mathrm{s}\rangle p(\mathbf{\Omega}\cdot\mathbf{\Omega}_0)$$

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source:
$$Q_S(ct,z,\mathbf{\Omega}) = F_0\delta\left(ct-\frac{z}{\mu_0}\right)\left|\dot{T}\left(\langle\sigma\rangle\frac{z}{\mu_0}\right)\right|\langle\sigma_\mathrm{s}\rangle p(\mathbf{\Omega}\cdot\mathbf{\Omega}_0)$$

Followed, after solution, by:

$$I_\mathrm{sca}(ct,z,\mathbf{\Omega}) = \begin{cases} \int_{\max\{0,z-ct\mu\}}^{z} S\left(ct-\frac{z-z'}{\mu},z',\mathbf{\Omega}\right)T\left(\langle\sigma\rangle\frac{z-z'}{\mu}\right)\mathrm{d}z'/\mu & \text{for } \mu>0 \\ \int_{z}^{\min\{H,z+ct|\mu|\}} S\left(ct-\frac{z'-z}{|\mu|},z',\mathbf{\Omega}\right)T\left(\langle\sigma\rangle\frac{z'-z}{|\mu|}\right)\mathrm{d}z'/|\mu| & \text{for } \mu<0 \end{cases}$$

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source:
$$Q_S(ct,z,\mathbf{\Omega}) = \overbrace{F_0\delta\left(ct-\frac{z}{\mu_0}\right)\left|\dot{T}\left(\langle\sigma\rangle\frac{z}{\mu_0}\right)\right|}^{\text{Directly transmitted from TOA, ...}}\underbrace{\langle\sigma_\mathrm{s}\rangle p(\mathbf{\Omega}\cdot\mathbf{\Omega}_0)}_{\text{... 1ce scattered,}}$$

Directly transmitted from TOA, …

… 1ce scattered,

Followed, after solution, by:

$$I_\mathrm{sca}(ct,z,\mathbf{\Omega}) = \begin{cases} \int_{\max\{0,z-ct\mu\}}^{z} S\left(ct-\frac{z-z'}{\mu},z',\mathbf{\Omega}\right)\overbrace{T\left(\langle\sigma\rangle\frac{z-z'}{\mu}\right)\mathrm{d}z'/\mu}^{} & \boxed{\text{for } \mu>0} \\ \int_{z}^{\min\{H,z+ct|\mu|\}} S\left(ct-\frac{z'-z}{|\mu|},z',\mathbf{\Omega}\right)T\left(\langle\sigma\rangle\frac{z'-z}{|\mu|}\right)\mathrm{d}z'/|\mu| & \text{for } \mu<0 \end{cases}$$

… and directly transmitted back to TOA ($z = H$).

Formulation of *generalized* RT in plane-parallel media

Parametric **GRT model:**

$$\begin{cases} T_a(\tau) = \left(1 + \dfrac{\tau}{a}\right)^{-a} \\ \left|\dot{T}_a(\tau)\right| = \left(1 + \dfrac{\tau}{a}\right)^{-(a+1)} \end{cases}$$

Standard **RT model is recovered at** $a \to \infty$

… the only case where $T_\infty(\tau) = |\mathrm{d}T_\infty/\mathrm{d}\tau|(\tau) = \exp(-\tau)$.

Singly-scattered radiance at TOA:

$$\mathrm{BRF}_a(\Omega_0,\Omega) = \frac{\pi I(0,\Omega)}{\mu_0 F_0} = \frac{\pi\varpi_0 p(\Omega\cdot\Omega_0)}{\mu_0|\mu|}\int_0^\tau |\dot{T}_a(\tau'/\mu_0)|T_a(\tau'/|\mu|)\mathrm{d}\tau'$$

$$\frac{\mathrm{BRF}_a(\Omega_0,\Omega)}{\varpi_0 4\pi p(\Omega\cdot\Omega_0)} = \frac{a(\mu_0|\mu|)^a}{4|\mu|(\mu_0-|\mu|)^{2a}}\left[B\left(1-\frac{|\mu|}{\mu_0},2a,1-a\right) - B\left(\frac{1-|\mu|/\mu_0}{1-\tau/a\mu_0},2a,1-a\right)\right]$$

$$= \frac{1-\mathrm{e}^{-(1/\mu_0+1/|\mu|)\tau}}{4(\mu_0+|\mu|)}$$, when $a \to \infty$

$B(x,a,b) = \int_0^x t^{a-1}(1-t)^{b-1}\mathrm{d}t$

Incomplete Euler Beta function

Formulation of *generalized* RT in plane-parallel media

***Parametric* GRT model:**

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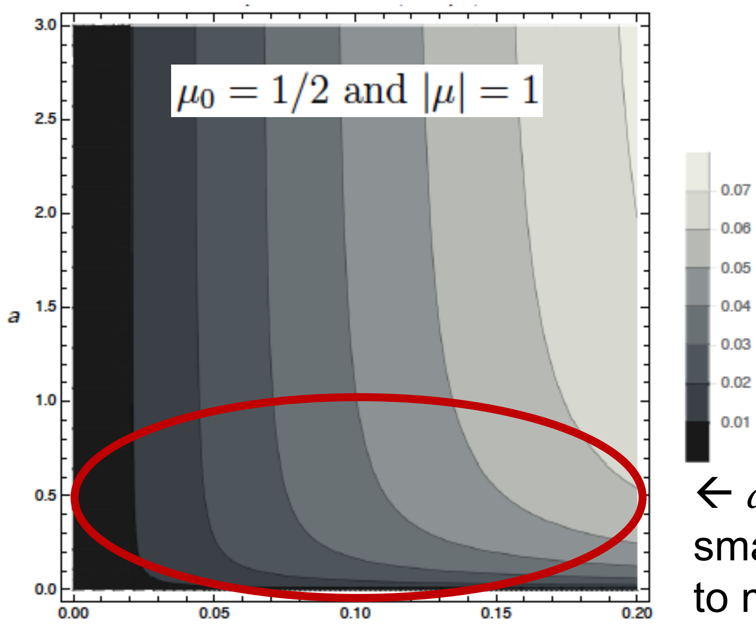
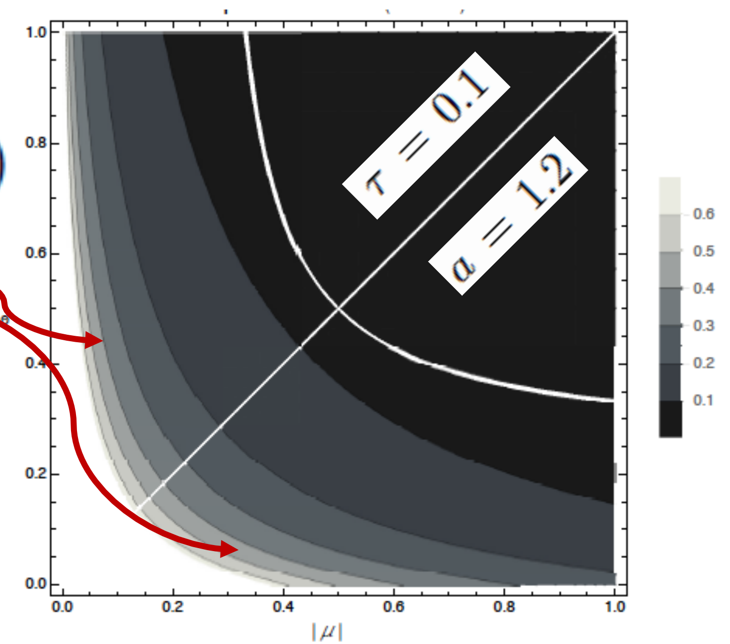
… the only case where $T_\infty(\tau) = |\mathrm{d}T_\infty/\mathrm{d}\tau|(\tau) = \exp(-\tau)$.



$$\frac{\mathrm{BRF}_a(\Omega_0,\Omega)}{\varpi_0 4\pi p(\Omega\cdot\Omega_0)}$$

reciprocity violation at small enough a and μ's

← a needs to be small (variance large) to make a difference!



Formulation of *generalized* RT in plane-parallel media

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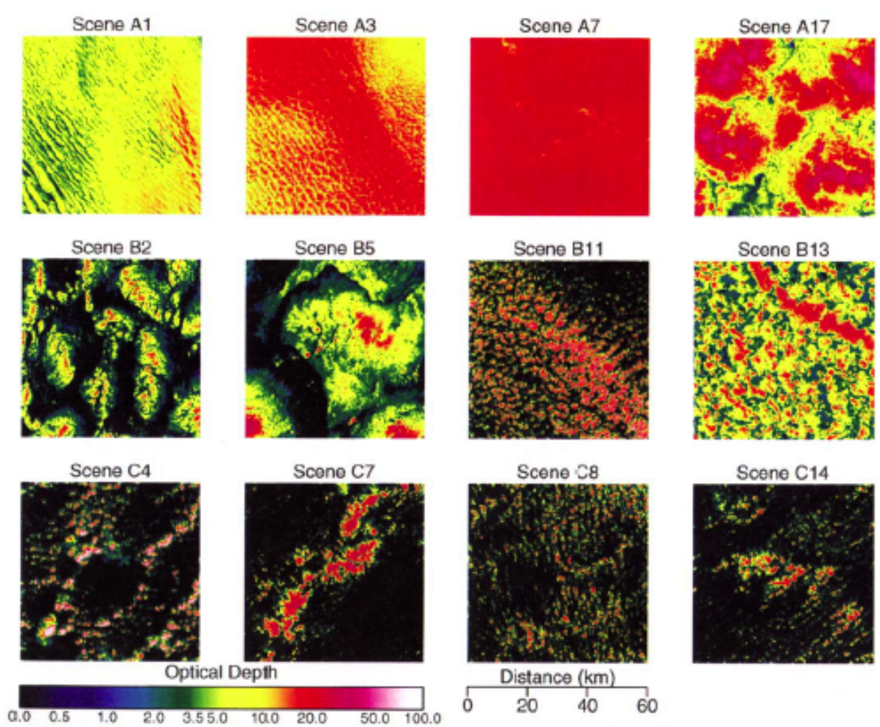
Standard **RT model is recovered at** $a \to \infty$

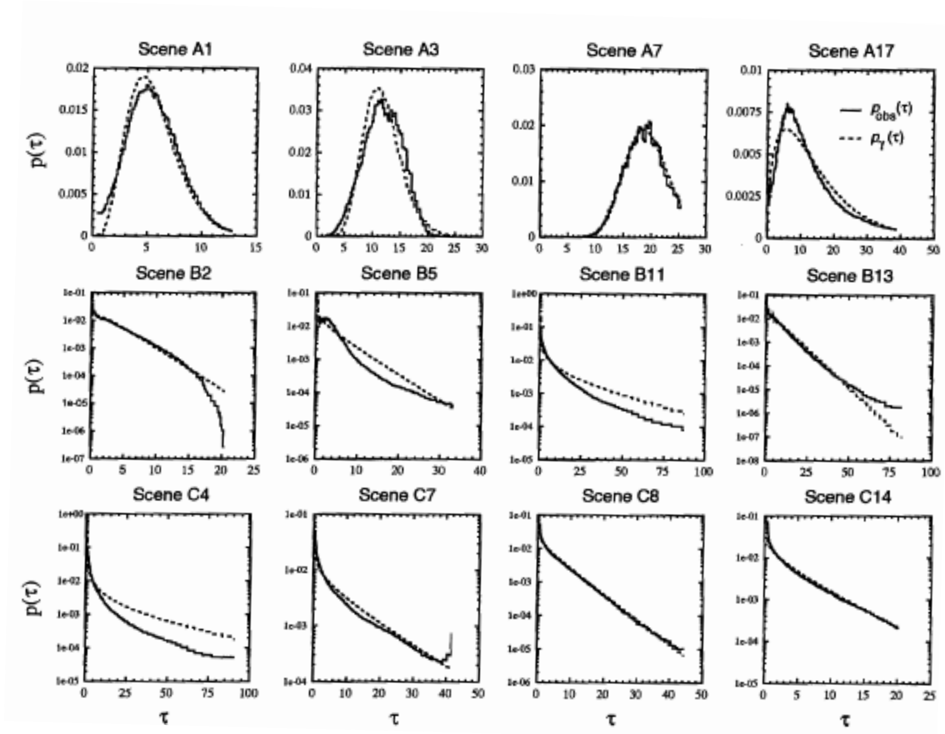
… the only case where $T_\infty(\tau) = |\mathrm{d}T_\infty/\mathrm{d}\tau|(\tau) = \exp(-\tau)$.

But, why mess with the <u>propagation</u> part of the transport kernel in the first place?

Motivation of *generalized* RT in plane-parallel media, 1:

- The turbulent nature of clouds ensures long-range correlations in fluctuating extinction field: structure functions ~r^{2H}, with $H \approx 1/3 > 0$.
- Hence scale-independence of extinction averaged over a segment of fixed length s; just need to know the stats of $\tau(s)$ at one representative value of s.





H. W. Barker, B. A. Wielicki, and L. Parker, A parameterization for computing grid-averaged solar fluxes for inhomogeneous marine boundary layer clouds - Part 2, Validation using satellite data, *J. Atmos. Sci.* **53**, 2304-2316 (1996).

Motivation of *generalized* RT in plane-parallel media, 1:

- The turbulent nature of clouds ensures long-range correlations in fluctuating extinction field: structure functions ~r^{2H}, with $H \approx 1/3 > 0$.
- Hence scale-independence of extinction averaged over a segment of fixed length s; just need to know the stats of $\tau(s)$ at one representative value of s.

$$p(\tau(s);\overline{\tau}(s),a) \approx \frac{1}{\Gamma(a)}\left(\frac{a}{\overline{\tau}(s)}\right)^{a} \tau(s)^{a-1}\mathrm{e}^{-a\tau(s)/\overline{\tau}(s)},$$

$$\text{where } a = \frac{1}{\overline{\tau(s)^2}\Big/\overline{\tau(s)}^2 - 1} \text{ and } \tau(s) = \int_0^s \sigma(\boldsymbol{x}+\boldsymbol{\Omega}s')\mathrm{d}s'$$

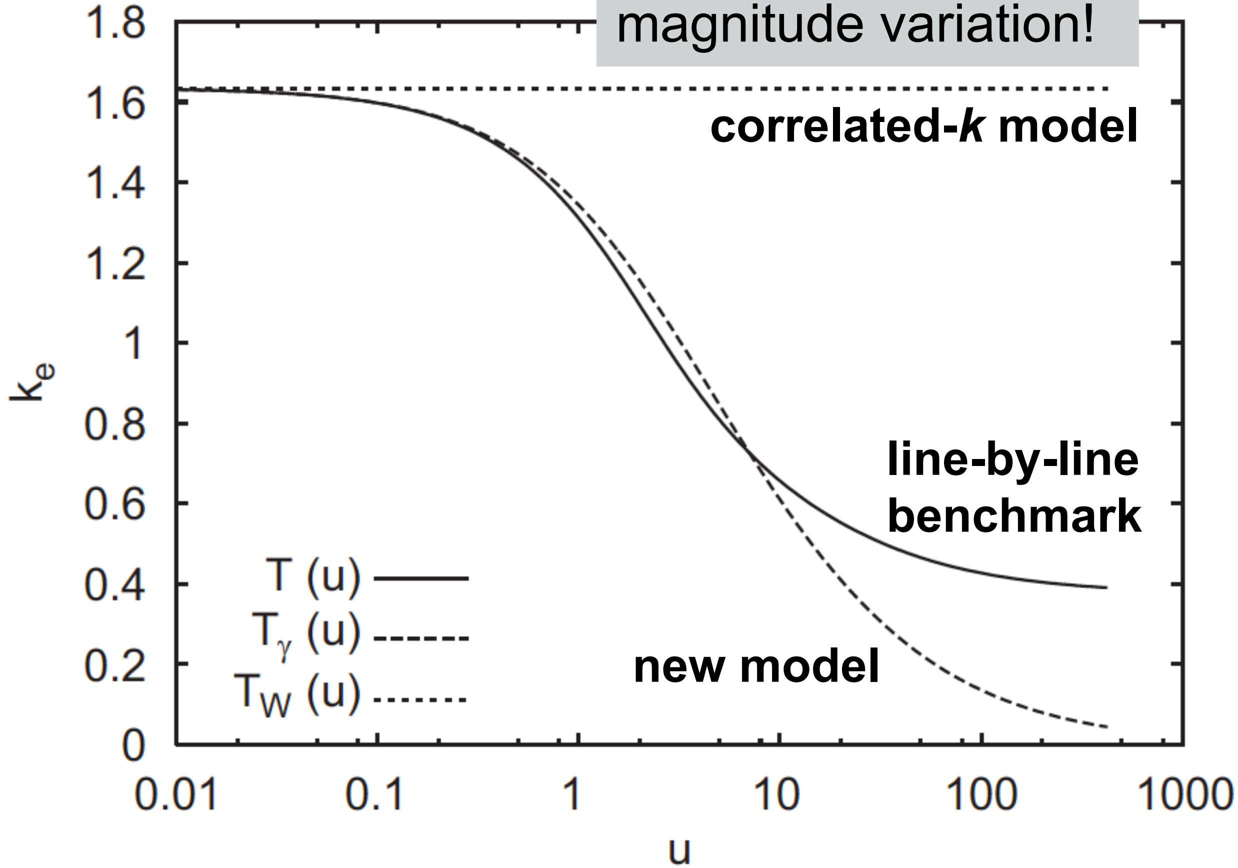
$$\text{Therfore } \overline{T_{\mathrm{dir}}(s)} = \overline{\mathrm{e}^{-\tau(s)}} = \int_0^\infty \mathrm{e}^{-\tau(s)} p(\tau(s);\overline{\tau}(s),a)\mathrm{d}\tau(s) = \frac{1}{\left(1+\frac{\overline{\tau(s)}}{a}\right)^{a}}$$

a is mean²/variance

Motivation of *generalized* RT in plane-parallel media, 2:

$$k_{e\gamma} = \frac{\ln(1+\langle k \rangle V^2 u)}{V^2 u}$$

H$_2$O at 0.7 to 5 μm in the stratosphere: 12 orders-of-magnitude variation!



$$T_\gamma(u) = \frac{1}{(1+\beta u)^\gamma}$$

where

$$\gamma = 1/V^2$$

$$\beta = \langle k \rangle V^2$$

$$V^2 = \frac{\langle k^2 \rangle}{\langle k \rangle^2} - 1$$

A. J. Conley and W. D. Collins, Extension of the weak-line approximation and application to correlated-*k* methods, *JQSRT* **112**, 1525-1532 (2011).

How to combine particle scattering and gaseous absorption in GRT?

Use equivalency of time-dependent RT and absorption by a uniform gas:

$$I_\lambda(z,\boldsymbol{\Omega}) \equiv \hat{I}(z,\boldsymbol{\Omega};k_\lambda) = \int_0^\infty \exp(-k_\lambda\, ct) I(ct,z,\boldsymbol{\Omega}) \mathrm{d}ct$$

In *standard* 1D RTE (integral or integro-differential forms):

$$\sigma = \sigma_\mathrm{s} + \sigma_\mathrm{a} = \omega_0 \sigma_\mathrm{p} + (1-\omega_0)\sigma_\mathrm{p} \rightarrow \sigma_\mathrm{a} = (1-\omega_0)\sigma_\mathrm{p} + k_\lambda$$

… a *local* extension

In *generalized* 1D RTE (integral form only!):

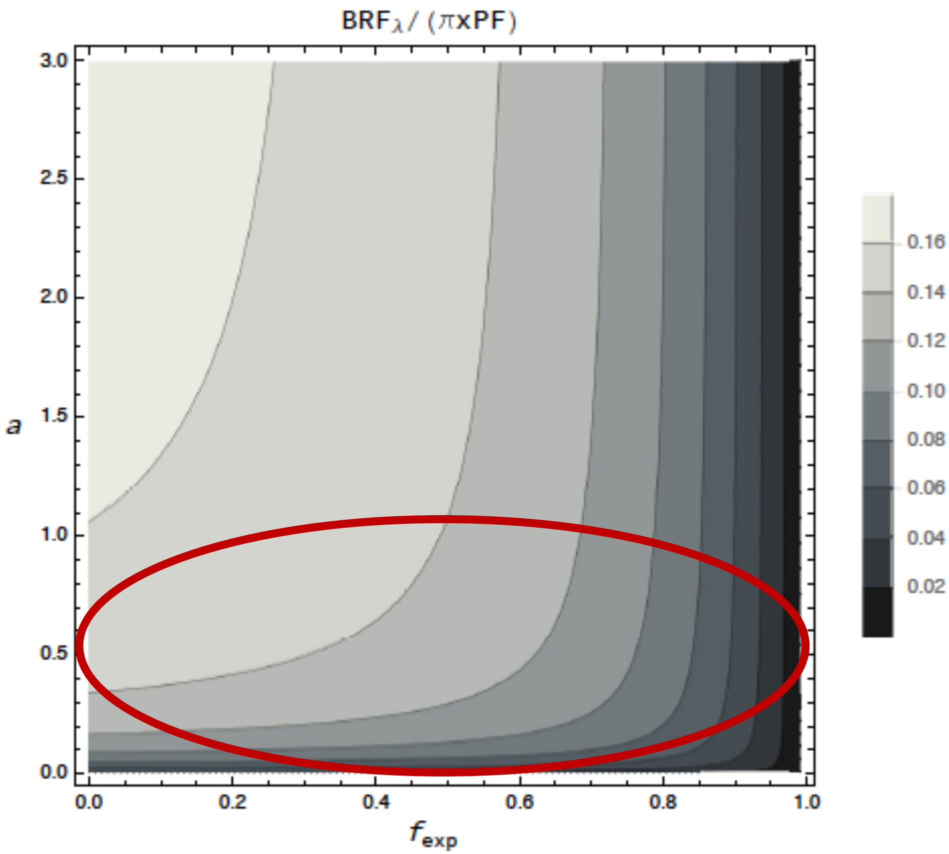
$T(\tau)$ and $\left|\dot{T}(\tau)\right|$ to be multiplied by: $\exp[-k_\lambda(z-z')/\mu]$

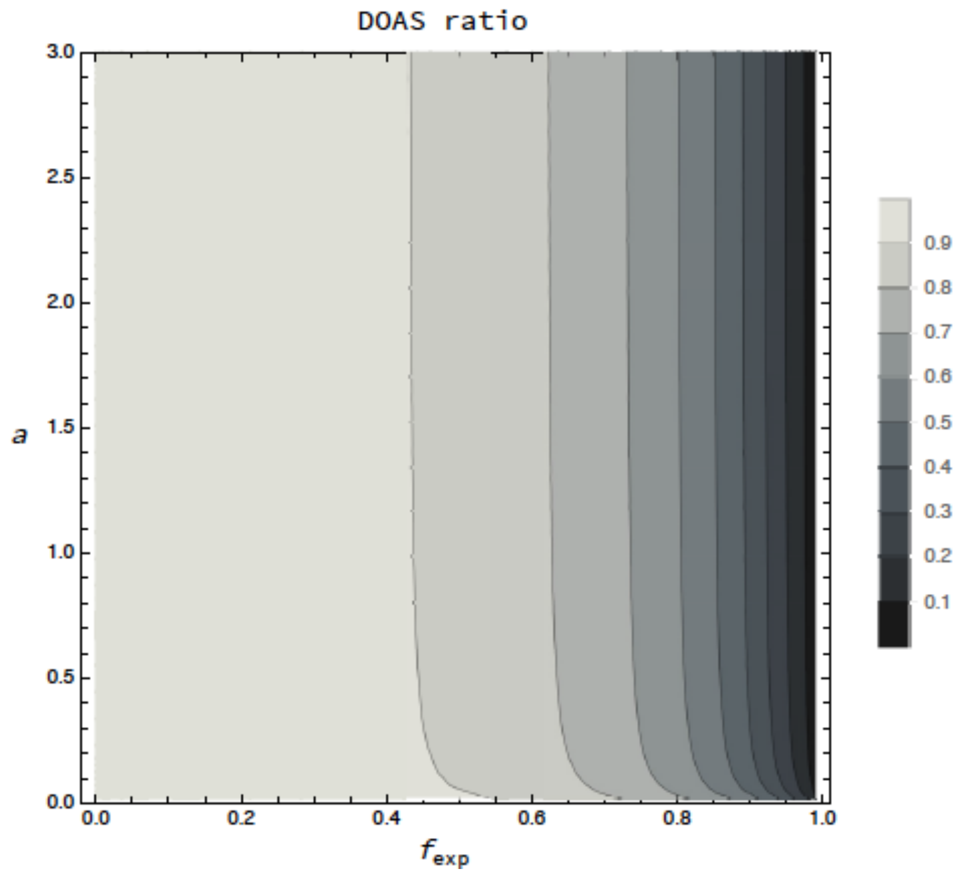
… a *non-local* extension

Subpixel spatially *heterogeneous* aerosol scattering in an absorbing gas: Monochromatic estimation

Noticeable impacts in BRF
(at small enough *a*)

… all but gone in DOAS ratio:
$BRF_{in\text{-}band}/BRF_{continuum}$



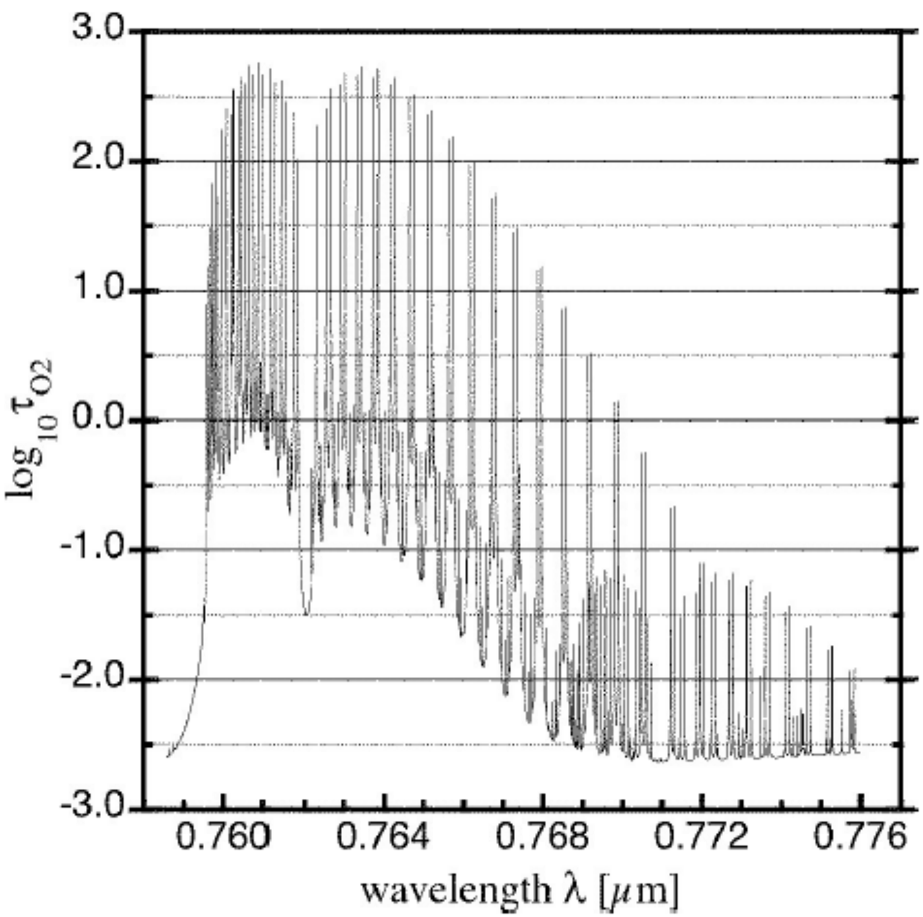


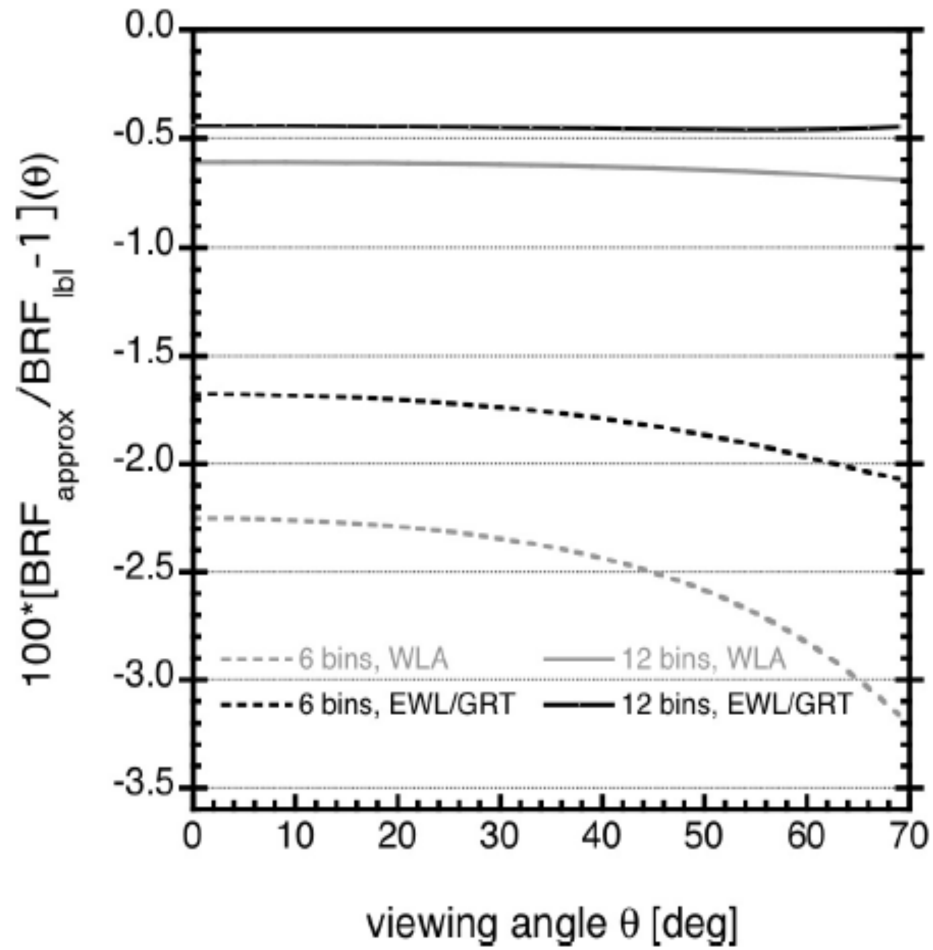
f_{exp} = (gaseous absorption) / (total extinction) coefficients

Subpixel spatially *homogeneous* aerosol scattering in an absorbing gas: Broadband estimation

N_λ = 29,620 single-scattering BRF evaluations in line-by-line benchmark computations.

N_{bin} = 6 or 12 single-scattering BRF evaluations in correlated-*k* or GRT estimations: % error ⬇





Summary & Outlook

- Rigorous extension of GRT to *combined* particle scattering and gaseous absorption
- *Analytical* solution in GRT for single-scattering, applicable to thin aerosol layers
- Application of GRT to *fast-but-accurate* spectral integration, including scattering
- <u>To do:</u> Incorporate into existing (Markov-chain) GRT multiple scattering code

<u>Details:</u>

A.B. Davis, F. Xu, D.J. Diner, Generalized radiative transfer theory for scattering by particles in an absorbing gas: Addressing both spatial and spectral integration in multi-angle remote sensing of optically thin aerosol layers, *JQSRT* **205**, 148–162 (2018).

A.B. Davis, F. Xu, D.J. Diner, Addendum to “[the above]”, *JQSRT* **206**, 251–253 (2018).